

Tetrahydrophthalic anhydride
85-43-8 | DTXSID3026516

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 29.9 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.63e-01

Confidence level: 7.09e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Phthalic anhydride</div> <div>Measured: 36.3</div> <div>Predicted: 38.0</div>	<div>Image not found</div> <div>2-Nitrobenzamide</div> <div>Measured: 28.2</div> <div>Predicted: 42.6</div>	<div>Image not found</div> <div>Phthalic acid</div> <div>Measured: 11.7</div> <div>Predicted: 21.4</div>
<div>Image not found</div> <div>3-Nitrobenzamide</div> <div>Measured: 89.1</div> <div>Predicted: 64.5</div>	<div>Image not found</div> <div>(2-Fluorophenyl)urea</div> <div>Measured: 20.9</div> <div>Predicted: 52.8</div>	